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From graphene to graphynes: Mechanical properties and fracture behavior

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Graphyne is another 2D allotrope of carbon similar to graphene. Graphyne consists of *sp* and sp^2 hybridized carbon atoms that are packed into a non-regular honeycomb crystal lattice. In this paper, graphene and four different graphynes (α, β, γ, and 6,6,12 graphynes) are investigated by the molecular dynamics simulation method with the view to explore their mechanical properties and fracture behavior under uniaxial and biaxial tensile loadings. It is found that the acetylenic linkages in graphyne structures have a strong effect on the mechanical properties and fracture behaviors of graphynes. The higher the percentage of the linkages in graphynes, the lower is the Young's modulus and fracture stress, which is attributed to the lower atoms density in graphynes and the weak single bonds in the acetylenic linkages. The crack of the graphynes is found to be initiated at the single bond of the acetylenic linkages in the structures. Among the four graphynes studied, the 6,6,12-graphyne shows the most obvious directional anisotropy in the mechanical properties.

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